TEMPERATURE CONTROL OF INDUSTRIAL GAS PHASE PROPYLENE POLYMERIZATION IN FLUIDIZED BED REACTORS USING MODEL PREDICTIVE CONTROL

Ahmad Shamiri[1], Mohamed Azlan Hussain[1], Farouq Sabri Mjalli[2], Arash Arami-Niya[1]

[1]Department of Chemical Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

ahmadshamiri@gmail.com

[2]Petroleum & Chemical Engineering Department, Sultan Qaboos University, Muscat 123, Oman

ABSTRACT

Two-phase dynamic model describing gas phase propylene polymerization in a fluidized bed reactor was used to explore the dynamic behavior and process control of the reactor temperature by manipulating the catalyst feed rate and reactor cooling water flow.

The analysis was performed using a two phase model, the presence of particles in the bubbles and the excess gas in the emulsion phase and consequently polymerization reaction in both phases were considered.

A model predictive control (MPC) technique is implemented to control of the nonlinear process and compared its performance with conventional PI controllers tuned using the Internal Model Control (IMC) method as well as the standard Ziegler-Nichols (Z-N) method.

The closed-loop simulations revealed that the Z-N PI controller produced oscillatory responses and the MPC and the IMC-Based PI controllers were able to track the changes in the set point. However the quality of the MPC set point tracking was superior to that of the IMC-Based PI controller.

INTRODUCTION

Modeling and control of the polymerization process in fluidized bed reactors such as polypropylene production are challenging issues in process and control engineering. This is mainly because of the high non-linearity of the process dynamics due to complicated reaction mechanisms, complex flow characteristics of gas and solids, various heat and mass transfer mechanisms and the interaction between the control loops. Many studies were reported for the modeling and control of olefin polymerization processes using various types of algorithms (Choi and Ray, 1985, Dadebo et al., 1997).

A process schematic of an industrial gas-phase fluidized bed polypropylene reactor is shown in Figure 1. To maintain acceptable polymer production rate which is an important goal for industry it is necessary to keep the reactor bed temperature above the dew point of the reactants to avoid gas condensation and below the melting point of the polymer to prevent particle melting and agglomeration and consequently reactor shut down.

Most of the reactor design and control problems are associated with achieving adequate production rate and heat removal from the reactor. The steady-state and dynamic behavior

of the reactor is influenced by many process variables such as the superficial gas velocity, feed gas temperature, monomer concentration, catalyst activity, catalyst feed rate, etc.
Choi and Ray (1985) used a dynamic model considering bubble and emulsion phases in the bed in the first attempt to describe the dynamics of polypropylene production. They showed that a PI feedback control scheme can be used to control the process transients, but it is limited by the recycle gas cooling capacity.
Dadebo *et al* (1997) showed that for the temperature control of industrial gas phase polyethylene reactors the nonlinear error trajectory controller (ETC) exhibits significantly superior responses in terms of speed, damping and robustness compared with an optimally-tuned PID controller over a wide range of operating conditions.
Due to the high nonlinearities and difficulties involved in the dynamics and control of the gas phase propylene polymerization fluidized bed reactor, an efficient process control scheme need to be implemented. However, it is beyond the capability of the conventional controller with fixed controller settings to achieve excellent control of the reactor variables. In order to achieve good control of the reactor variables, a more intelligent and efficient process control scheme is needed where the controller is able to automatically re-design itself in real time according to the changing process dynamics.

In the present study, a two-phase model with comprehensive kinetics for propylene homo-polymerization in a fluidized bed reactor that considers the presence of particles in the bubbles and the excess gas in the emulsion phase with polymerization reaction in both phases (Shamiri *et al*., 2011, Cui *et al*., 2000, Cui *et al*., 2001) is considered. A Model Predictive Control (MPC) algorithm is used for controlling the reactor temperature by manipulating the coolant flow rate.

MATHEMATICAL MODELING OF PROPYLENE POLYMERIZATION

In the present study, the kinetic model of propylene homo-polymerization over a Ziegler-Natta catalyst based on the kinetic model developed by Shamiri *et al* (2010, 2011) and the dynamic two-phase flow structure proposed by Cui *et al* (2000, 2001) were combined and implemented to provide a more realistic understanding of the phenomena encountered in the bed hydrodynamics.

For details of the kinetic scheme, definitions of pseudo-kinetic rate constants and the correlations required for estimating the bubble volume fraction in the bed, the voidage of the emulsion phase and bubble phases, the emulsion phase and bubble phases gas velocities and mass and heat transfer coefficients for two-phase model, the reader is referred to a paper by Shamiri *et al* (2011).

The following dynamic material balances were written for all of the components in the bed.
For bubbles:

$$[M_i]_{b,(in)} U_b A_b - [M_i]_b U_b A_b - R_v \varepsilon_b [M_i]_b - K_{be}([M_i]_b - [M_i]_e) V_b - (1-\varepsilon_b)\frac{A_b}{V_{PFR}}\int R_{i_b}\, dz$$
$$= \frac{d}{dt}\left(V_b \varepsilon_b [M_i]_b\right) \tag{1}$$

For emulsion:

$$[M_i]_{e,(in)} U_e A_e - [M_i]_e U_e A_e - R_v \varepsilon_e [M_i]_e + K_{be}([M_i]_b - [M_i]_e) V_e \left(\frac{\delta}{1-\delta}\right) - (1-\varepsilon_e) R_{i_e}$$
$$= \frac{d}{dt}\left(V_e \varepsilon_e [M_i]_e\right) \tag{2}$$

The direction of mass transfer was assumed to be from bubble to emulsion phase. Furthermore, the energy balances can be expressed as:

For bubbles:

$$U_b A_b (T_{b,(in)} - T_{ref}) \sum_{i=1}^{m} [M_i]_{b,(in)} C_{pi} - U_b A_b (T_b - T_{ref}) \sum_{i=1}^{m} [M_i]_b C_{pi}$$
$$- R_v (T_b - T_{ref}) \left(\sum_{i=1}^{m} \varepsilon_b C_{pi} [M_i]_b + (1-\varepsilon_b)\rho_{pol} C_{p,pol} \right) + (1-\varepsilon_b) \frac{A_b \Delta H_R}{V_{PFR}} \int R_{pb}\, dz$$
$$+ H_{be}(T_e - T_b) V_b - V_b \varepsilon_b (T_b - T_{ref}) \sum_{i=1}^{m} C_{pi} \frac{d}{dt}([M_i]_b)$$
$$= \left(V_b (\varepsilon_b \sum_{i=1}^{m} C_{pi} [M_i]_b + (1-\varepsilon_b)\rho_{pol} C_{p,pol}) \right) \frac{d}{dt}(T_b - T_{ref}) \tag{3}$$

For emulsion:

$$U_e A_e (T_{e,(in)} - T_{ref}) \sum_{i=1}^{m} [M_i]_{e,(in)} C_{pi} - U_e A_e (T_e - T_{ref}) \sum_{i=1}^{m} [M_i]_e C_{pi}$$
$$- R_v (T_e - T_{ref}) \left(\sum_{i=1}^{m} \varepsilon_e C_{pi} [M_i]_e + (1-\varepsilon_e)\rho_{pol} C_{p,pol} \right) - (1-\varepsilon_e) R_{pe} \Delta H_R$$
$$- H_{be} V_e \left(\frac{\delta}{1-\delta}\right)(T_e - T_b) - V_e \varepsilon_e (T_e - T_{ref}) \sum_{i=1}^{m} C_{pi} \frac{d}{dt}([M_i]_e) =$$
$$\left(V_e (\varepsilon_e \sum_{i=1}^{m} C_{pi} ([M_i]_e) + (1-\varepsilon_e)\rho_{pol} C_{p,pol}) \right) \frac{d}{dt}(T_e - T_{ref}) \tag{4}$$

The initial conditions for solution of the model equations are as follows:

$$\left[M_i\right]_{b,t=0} = \left[M_i\right]_{in} \quad and \quad T_b(t=0) = T_{in} \tag{5}$$

$$\left[M_i\right]_{e,t=0} = \left[M_i\right]_{in} \quad and \quad T_e(t=0) = T_{in} \tag{6}$$

NONLINEAR MODEL PREDICTIVE CONTROL SCHEME (NMPC)

Nonlinear model predictive control (NMPC) is an optimization-based control strategy which is well suited for constrained and multivariable processes, the MPC controller predicts the future behavior of the actual system over a time interval defined by the

prediction horizon. In this study a dynamic process model is used in MPC in order to predict the controlled variable, in this system a process model is used in parallel to the plant.
A usual MPC formulation solves the following online optimization:

$$J = \Gamma_y \sum_{i=1}^{P} \left[Y(t+i) - R(t+i) \right]^2 + \Gamma_u \sum_{i=1}^{M} \left[\Delta u(t+i-1) \right]^2$$

Where J is the cost function to be minimized and Γ_y and Γ_u are the input and output weighting parameters and $R = [r(t+1), \ldots, r(t+P)]^T$ is a vector of the future setpoint and $\Delta u = [u(t), u(t+1), \ldots, u(t+M-1)]^T$ is a vector of manipulated variable values of length M. $Y = [Y(t+1), \ldots, Y(t+P)]^T$ includes the predicted outputs over the future horizon P, where y is the output vector. The controller moves horizon (M) and the prediction horizon (P) are used to adjust the speed of the response and hence to stabilize the feedback behavior. Γ_y is usually used for trade-off between different controlled outputs and Γ_u is used to penalize different inputs and thus to stabilize the feedback response.
Depending on the problem formulation, the controller parameters such as sampling time, control horizon, prediction horizon, and weighting matrices in the optimization formulation can be used to tune the performance of the predicted output.
In this study Y represents the emulsion phase temperature which is the controlled variable and variable u represents the cooling water flow rate.
The presented mathematical model for the gas phase propylene polymerization fluidized bed reactor consists of cooling water flow rate (F_{cw}) as a manipulated variable and emulsion phase temperature (T_e) as a controlled variable.
A model-predictive controller was designed using the MPC toolbox GUI and implemented in simulink using the MPC simulink block.

RESULTS AND DISCUSSION

The process was simulated at the operating conditions shown in Table 1.
The closed loop performance of the MPC scheme in tracking series of setpoint changes for the emulsion phase temperature in the polymerization reactor is evaluated. For this purpose, series of setpoint changes in opposite directions were introduced. The magnitude of the setpoints introduced for this loop was typical of the respective nominal operating range. For comparison purposes, conventional PI controllers tuned using the IMC (Chien and Fruehauf, 1990) method and the standard Z-N (Ziegler and Nichols, 1942) method, were included in this simulation. Both the IMC and Z-N PI controller tuning parameters were calculated based on analyses of the open loop process reaction curve for a particular operational region of the process.
To ensure good performance of the MPC controller, the tuning parameters must be appropriately tuned. Although Shridhar and Cooper (1997) suggestion were good starting values for tuning the controller parameter but the exact values used in this work were the result of further fine tuning based on actual control performance. In addition to the selection of controller tuning parameters, the values were chosen for the constraints and

imposed on loop are based on practical considerations acquired through real operational experience of the authors.
The resulting controller had a sampling time of 10 sec, a prediction horizon of 17, a control horizon of 1, an output variables weight of 0.09, and a manipulated variables weight of 0.008.
Figs. 3 and 4 show the performance of the MPC as compared to the IMC and Z-N PI controllers in tracking series of setpoint changes for the temperature loop as well as the corresponding controller moves. From Fig. 3, the failure of the Z-N PI controller to track the changes in the setpoints for the temperature loop was obvious. The Z-N PI controller produced oscillatory responses. Furthermore, as shown in Fig. 4, the controller moves observed were vigorous. However the shortcomings exhibited by the Z-N PI controller were not observed for the cases of MPC and the IMC-Based PI controllers. In general, both the MPC and the IMC-Based PI controllers were able to track the changes in the set point. However, the quality of the set point tracking as demonstrated by the MPC was superior to the IMC-Based PI controller in terms of their ability to attain minimal overshoot. Moreover, the MPC was able to not only produce controller moves which were well within the specified input constraints, but also the controller moves produced were non-aggressive and smooth for practical implementations. These were attributed to the ability of the MPC to handle constraints in the inputs, of which the conventional PI controller was unable to achieve. To summarize, Table 2 shows the Integral Absolute Error (IAE) for the three controllers in tracking the series of set point changes. The values of the IAE calculated were consistent with the previous discussions, where the performance of the MPC was superior to the conventional PI controllers.

CONCLUSIONS

Two-phase dynamic model describing gas phase propylene polymerization in a fluidized bed reactor was used to control the reactor temperature. The hydrodynamics of the fluidized bed reactor of polypropylene production was based on the dynamic two-phase concept of fluidization.
Two control algorithms namely, the conventional Proportional-Integral (PI) and model predictive controller (MPC) were tested for the stabilization of the process.
The MPC was compared to the conventional PI controller tuned using the Internal Model Control (IMC) method as well as the standard Ziegler-Nichols (Z-N) method in terms of setpoints tracking for the temperature loop as well as the corresponding controller moves.
The closed-loop simulations revealed that the Z-N PI controller produced an oscillatory response while the MPC and the IMC-Based PI controller were able to track the changes in the setpoint. However, the quality of the setpoint tracking as demonstrated by the MPC was superior to that of the IMC-Based PI controller in terms of the ability to attain minimal overshoot. Moreover, the MPC was able to not only produce controller moves which were well within the specified input constraints, but also the controller moves produced were non-aggressive and smooth for practical implementations. The values of the IAE calculated for the temperature loop indicate that the performance of the MPC was superior to the conventional PI controllers.

Tab. 1: Operating conditions and physical parameters considered in this work for modeling fluidized bed polypropylene reactors.

Operating conditions	**Physical parameters**
$V\ (m^3)=50$	$\mu\ (Pa.s)=1.14\times10^{-4}$
$T_{ref}\ (K)=353.15$	$\rho_g\ (kg/m^3)=23.45$
$T_{in}\ (K)=317.15$	$\rho_s\ (kg/m^3)=910$
$P\ (bar)=25$	$dp\ (m)=500\times10^{-6}$
Propylene concentration $(kmol/m^3)=0.9$	$\varepsilon_{mf}=0.45$
Hydrogen concentration $(kmol/m^3)=0.015$	
Catalyst feed rate $(kg/s)=0.0003$	

Tab. 2: Integral absolute error (IAE) for the MPC, IMC-Based PI controller, and the Z-N PI controller in tracking series of setpoint changes for the emulsion phase temperature.

Controller	IAE
MPC	2527
IMC-Based PI Controller	2712
Z-N PI Controller	4655

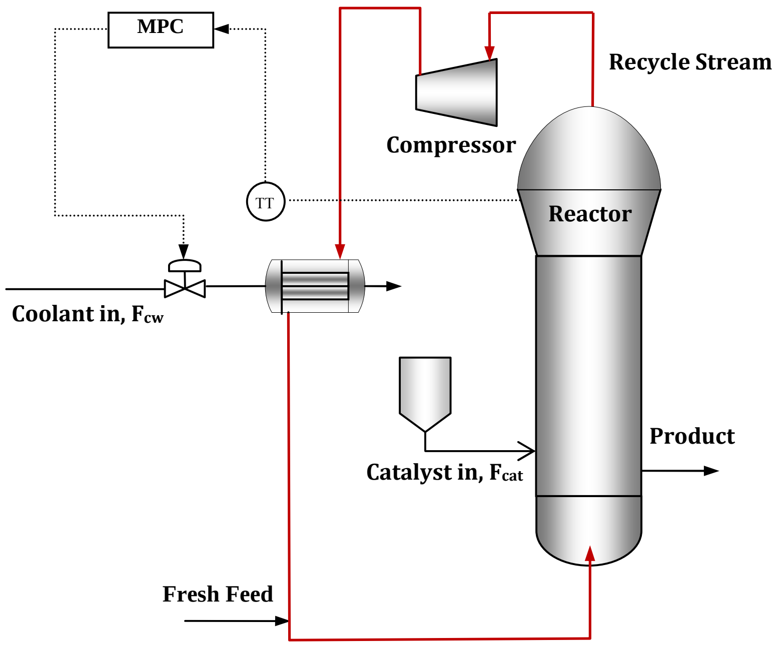


Fig. 1: Simplified schematic of the MPC design on the gas phase propylene polymerization fluidized bed reactor.

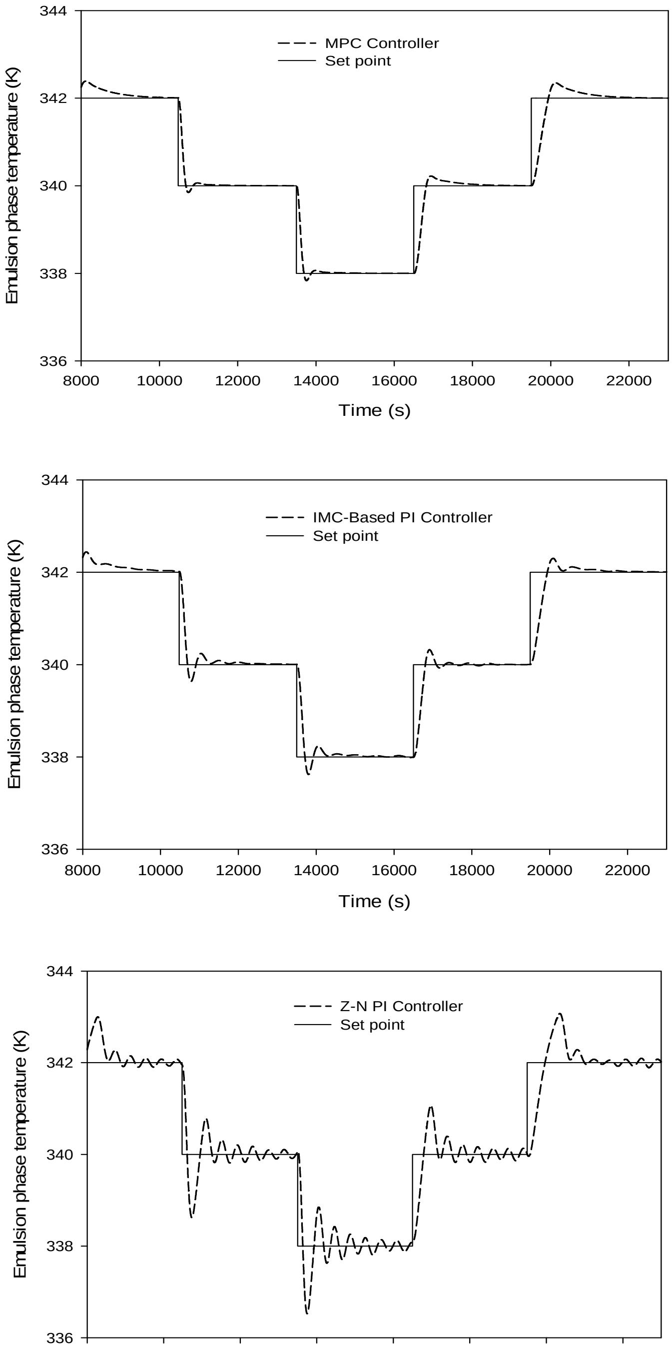
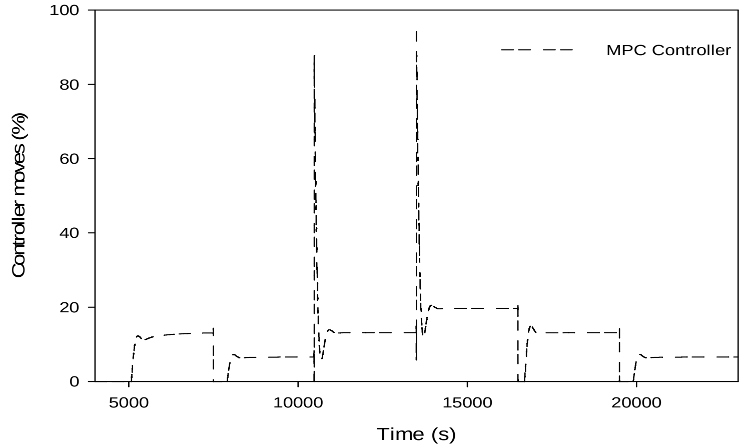
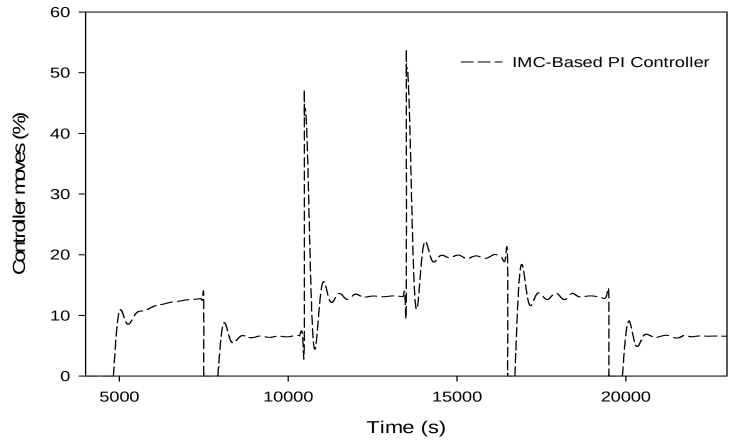


Fig. 3: Comparison of the performance between the MPC, IMC-Based PI controller (K_c = -18.5345, τ_I = 858.0787, τ_D = 0), and the Z-N PI controller (K_c = -33.3620, τ_I = 266.4696, τ_D = 0) in tracking series of setpoint changes in the emulsion phase temperature (T_e) (U_0=0.45m/s, F_{cat}=0.0003kg/s).


MPC Controller
Controller moves (%)
100
80
60
40
20
0
5000
10000
15000
20000
Time (s)


IMC-Based PI Controller
Controller moves (%)
60
50
40
30
20
10
0
5000
10000
15000
20000
Time (s)

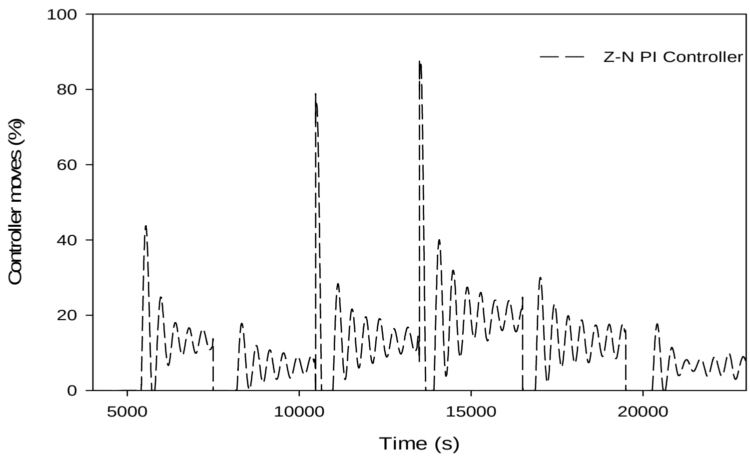

Z-N PI Controller
Controller moves (%)
100
80
60
40
20
0
5000
10000
15000
20000
Time (s)

Fig. 4: Comparison of the corresponding controller moves between the MPC, IMC-Based PI controller, and the Z-N PI controller for the emulsion phase temperature.

NOMENCLATURE

A	cross sectional area of the reactor, (m^2)
C_{pi}	specific heat capacity of component i (J/kg.K)
C_{pg}	specific heat capacity of gaseous stream (J/kg.K)
$C_{p,pol}$	specific heat capacity of solid product (J/kg.K)
d_b	bubble diameter (m)
d_p	particle diameter (m)
D_t	reactor diameter (m)
F_{cat}	catalyst feed rate (kg/s)
F_{cw}	cooling water flow rate (kg/s)
H	height of the reactor, (m)
H_{be}	bubble to emulsion heat transfer coefficient, ($W/m^3.K$)
K_{be}	bubble to emulsion mass transfer coefficient, (s^{-1})
M	monomer (propylene)
$[M_i]$	concentration of component *i* in the reactor ($kmol/m^3$)
$[M_i]_{in}$	concentration of component *i* in the inlet gaseous stream
R_p	production rate (kg/s)
R_i	instantaneous rate of reaction for monomer *i* (kmol/s)
R_v	volumetric polymer phase outflow rate from the reactor (m^3/s)
T	temperature of the gas entering the exchanger, (K)
T_{in}	temperature of the inlet gaseous stream, (K)
T_{wi}	temperature of the cooling water entering the heat exchanger, (K)
U_0	superficial gas velocity (m/s)
U_b	bubble velocity (m/s)
U_e	emulsion gas velocity (m/s)
U_{mf}	minimum fluidization velocity (m/s)
V_b	volume of the bubble phase
V_e	volume of the emulsion phase
V_{PFR}	volume of PFR

Greek letters

ΔH_R	heat of reaction (J/kg)
δ	volume fraction of bubbles in the bed
ε_b	void fraction of bubble for Geldart B particles
ε_e	void fraction of emulsion for Geldart B particles
ε_{mf}	void fraction of the bed at minimum fluidization
ρ_g	gas density (kg/m^3)
ρ_{pol}	polymer density (kg/m^3)

Subscripts and superscripts

b	bubble phase

e emulsion phase
i component type number
ref reference condition

REFERENCES

Ali, M. A.-H., Betlem, B., Weickert, G. & Roffel, B. (2007) Non-linear model based control of a propylene polymerization reactor. *Chemical Engineering and Processing,* 46**,** 554-564.

Chien, I. L. & Fruehauf, P. S. (1990) Consider IMC tuning to improve controller performance. *Chemical Engineering Progress,* 86**,** 33-41.

Choi, K. Y. & Ray, W. H. (1985) The dynamic behavior of fluidized bed reactors for solid catalysed gas phase olefin polymerization. *Chemical Engineering Science,* 40**,** 2261-2279.

Cui, H., Mostoufi, N. & Chaouki, J. (2000) Characterization of dynamic gas-solid distribution in fluidized beds. *Chemical Engineering Journal,* 79**,** 133-143.

Cui, H., Mostoufi, N. & Chaouki, J. (2001) Gas and solids between dynamic bubble and emulsion in gas-fluidized beds. *Powder Technology,* 120**,** 12-20.

Dadebo, S. A., Bell, M. L., Mclellan, P. J. & Mcauley, K. B. (1997) Temperature control of industrial gas phase polyethylene reactors. *Journal of Process Control,* 7**,** 83-95.

Shamiri, A., Azlan Hussain, M., Sabri Mjalli, F., Mostoufi, N. & Saleh Shafeeyan, M. (2011) Dynamic modeling of gas phase propylene homopolymerization in fluidized bed reactors. *Chemical Engineering Science,* 66**,** 1189-1199.

Shamiri, A., Hussain, M. A., Mjalli, F. S. & Mostoufi, N. (2010) Kinetic modeling of propylene homopolymerization in a gas-phase fluidized-bed reactor. *Chemical Engineering Journal,* 161**,** 240-249.

Shridhar, R. & Cooper, D. J. (1997) A Tuning Strategy for Unconstrained SISO Model Predictive Control. *Industrial and Engineering Chemistry Research,* 36**,** 729-746.

Ziegler, J. G. & Nichols, N. B. (1942) Optimum settings for automatic controllers. *Transactions of the ASME,* 64**,** 759-768.

BRIEF BIOGRAPHY OF PRESENTER

Ahmad Shamiri:

I have been working at the Razi Petrochemical Company as a process and production engineer for 9 years. I’m currently PhD student in the field of process modeling and control at the University of Malaya.